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# INDIRECT MEASUREMENTS OF ATMOSPHERIC TEMPERATURE PROFILES FROM SATELLITES: I. INTRODUCTION

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ABSTRACT

Artificial earth satellites offer a unique opportunity to exploit the possibility of deducing temperature profiles on a global scale from measurements of radiance in several narrow spectral intervals in a strongly absorbing band of an atmospheric gas whose mixture is uniform. In the earth's atmosphere the 4.3-micron and 15-micron bands of carbon dioxide and the 5-mm. band of oxygen may be used; only the 15-micron band is considered in detail, although the procedures are applicable to the other bands. The problem considered is the numerical solution of the integral form of the radiative transfer equation from measurements in a finite set of spectral intervals. It is shown that, by a suitable approximation of the Planck radiance, the radiative transfer equation can be reduced to an integral equation of the first kind. After a discussion of the kernel, which is associated with the transmittance of the gas, the equation is changed to a finite set of equations which is amenable to numerical solution. The solution is limited to about six pieces of information, which may be expressed as points along the vertical profile, or as coefficients of an expansion; the limitation in information is manifest in the transmittance curves for the several spectral intervals, the errors of measurement, and the approximations employed. However, even in this limited case the formal solution of the set of equations is unstable. A method of stabilizing the solution by smoothing is discussed. In this process the amount of smoothing remains small, so that the inherent properties of the temperature profile are not affected. Several possible forms of the solution are discussed, and it is concluded that empirical orthogonal functions are preferred because they contain the physical information lacking in analytical forms. Examples are shown of solutions for radically different profiles, both with "exact" simulated measurements and with random errors introduced.

## 1. BACKGROUND

In recent years the reality of artificial earth satellites has excited interest in the prospects of deducing atmospheric parameters from radiometric measurements taken from orbiting vehicles. The concept of determining the state of an atmosphere from spectral measurements is not new; since 1905, when Schuster first conceived the radiative transfer equation, astrophysicists have developed a copious literature on the interpretation of the spectra of the sun and the stars. However, their task has been enormously complicated by the lack of specific a priori knowledge of the relative abundances of the elements, by the high degree of dependence of the spectral transmittance upon the state itself, by inexact knowledge of the transitions probabilities of the different species composing the stellar atmospheres, and by other problems such as departures from local thermodynamic equilibrium. Because of a multiplicity of unknowns, the only technique available was a sort of analog method by which model atmospheres were postulated and direct solutions of the radiative transfer equation were carried out to reproduce best the observed spectra.

In the case of planetary atmospheres, attention until very recently has been confined largely to the photographic region (0.3 to 1.2 microns), in which the absorbing gases do not contribute to the source function. By measuring the amount of absorption by spectral lines of these cool gases, relatively crude estimates could be made of the amount of the gas and the total amount of atmosphere estimated, as in the case of Mars (see Kaplan et al. [26]).

When the earth is viewed from an orbiting artificial satellite, the problems which are so formidable with the sun, stars, and planets are greatly simplified. The total amount of atmosphere is known within 1 percent or better over the greater part of the globe, and the absorptance by the atmospheric gases is also well known. Several gases, including molecular oxygen (see Byers [3]) and carbon dioxide (Hagemann et al. [21]) are known to be uniformly mixed up to altitudes of 30 km., which are of primary meteorological interest, and doubtlessly to more than twice that height, above which dissociation by solar irradiation destroys this uniformity. It has been shown (Curtis and Goody [6]) that local thermodynamic equilibrium exists below about 70 km., and one is therefore free to employ the classical relations of the Planck function, Kirchhoff's law, and the Stefan-Boltzmann relation. The molecular transitions in the infrared and microwave regions arise mostly from states near the ground levels, and transmittances are therefore only weakly dependent upon temperature under terrestrial conditions (200°–300° K.). Finally, scattering by the aerosols in the atmosphere is negligible in the infrared and microwave regions, except for water droplets and ice crystals (Deirmendjian [7] and Zdunkowski et al. [56]).

With the above favorable conditions in mind, King [27] gave a brief and general statement regarding the possibility of applying satellite measurements to the integral transform (the integral form of the radiative transfer equation) to deduce vertical profiles of atmospheric parameters. Shortly thereafter, Kaplan [25] made a more specific proposal to measure the atmospheric radiance in ten narrow spectral intervals in the 15-micron band of carbon dioxide, and, by an inversion of the integral transform, to deduce the vertical temperature profile of the atmosphere. It is this latter proposal which will be pursued in this and the following papers.

The United States Weather Bureau (more recently in the role of the National Environmental Satellite Center), in cooperation with the National Aeronautics and Space Administration, has engaged in an active program to produce an infrared spectrometer capable of making measurements necessary for the deduction of the vertical temperature profile and suitable for eventual use aboard a satellite. The experiment was simplified, at the suggestion of S. Fritz, to include only those measurements required to determine the atmospheric temperature profile in the stratosphere. A "breadboard" model of the proposed instrument was produced (Dreyfus and Hilleary [9] and Dreyfus [8]), tested, and used to conduct experiments discussed in later papers of this series. Following the success of this instrument, advanced instruments were produced to be flown on balloons and to serve as interim development models of a satellite spectrometer. One of these instruments has been flown and the results are reported in a later paper of this series.

Other instruments may be used for the temperature determination. For example, Suomi [48] has suggested a pneumatic detector for the 15-micron carbon dioxide band. Houghton [24] has suggested scanning lines of the carbon dioxide band by means of a variation of the spacing of a Fabry-Perot interferometer. A spectral scan can also be achieved with a Michelson interferometer; Hanel and Chaney [22], Saiedy [43], and others are working on the development of such an instrument. A promising instrumental approach has been suggested by Smith and Pidgeon [47], in which they use a combination of filters and a carbon dioxide gas-cell chopper. However, the conservative but large spectrometer now being prepared for a Nimbus satellite is the only instrument which has been fully developed at this time to perform the measurements required for the temperature profile determination.

Following the decision to proceed with the instrumental program, several studies were conducted to test the reliability of the technique, to determine the instrumental requirements, and to develop the mathematical basis for the solution. Wark [54] and Yamamoto [55] made some initial attempts to resolve some basic difficulties; however, these studies were confined to three and four spectral intervals, respectively, and with the expansion of the number of intervals to six in the balloon instrument and to seven in the satellite instrument, the inherent instability in the solution became a matter of primary concern.

Singer [44] had made a similar proposal to determine the ozone distribution in the atmosphere from scattered sunlight in the ultraviolet Hartley band; this was followed by a further discussion by Singer and Wentworth [45]. Later, Twomey [49] discussed this same problem; however, in subsequent numerical solutions, he, like all others who have ventured into the field of numerical inversion of integral transforms, found the solution to be unstable and, therefore, physically meaningless. He found, however, that the solutions could be stabilized by the pragmatic device of adding to $N$ linear equations, with $N$ unknowns, $N$ relations, equating each of the unknowns to some expected value and solving the overdetermined system by least squares procedure (in which a very small weight was assigned to the additional restraint equations). The timely appearance of the paper by Phillips [41] permitted a more formal basis to be found for this method, which has been refined and developed (Twomey [50], [51], and Twomey and Howell [52]). It is this work which forms the basis for the solution of the temperature profile problem. Twomey discusses the problem in the next paper of this series.

This discussion would not be complete without reference to other work on this problem. King [28], [29] has discussed the inversion problem, and has taken a different approach to the method of solution. Marchuk [35] has published a discussion which has solved the problem only in a formal sense. Malkevitch and Tamarskii [34], on the other hand, have devised a technique of expanding temperature differences from a mean sounding in terms of empirical orthogonal functions (Obukhov [40]), which is similar in some respects to the method employed later in this paper, but must, of necessity, fall short of the objective without some sort of smoothing. McClachey [38], working with the 4.3-micron band, has employed an iteration technique similar to that of Malkevitch but not using empirical functions. An interesting application of the smoothing technique has been applied by Krakow [30] in determining the temperature structure of hot flames from measurements in the 4.3-micron band. Fryberger and Uretz [19] have also published on the topic of indirect temperature soundings.

As suggested above, measurements in other bands in the microwave and the infrared regions may be used for the purpose of deducing temperature profiles. Kaplan and his associates are concerning themselves with the 4.3-micron band of carbon dioxide; this band is stronger than the 15-micron band and therefore has certain advantages in sounding the stratosphere. Meeks and Lilly [39] and Smith [46] have suggested conducting measurements in the 5-mm. spin-reorientation band of oxygen; this band has the advantages over the infrared bands of having enormously greater resolution by means of coherent detectors, and of being undisturbed by the presence of thin clouds which affect the infrared region. The deduction of temperature profiles from microwave measurements has been discussed extensively by Fow [16]. Fischbach [13] has suggested measurements of the refraction of stars through the atmosphere as an alternate sounding technique.

Of interest is another method of obtaining the vertical ozone distribution. Frith [18] suggested that the ozone could be inferred by observing the sun in the ultraviolet Hartley band; as the satellite moves in its orbit the sun is occulted by the ozone layer, and from the changing output of the detector related to the position of the sun and the satellite, the ozone distribution can be inferred. This experiment was flown in the UK–II satellite, but no results have been published. Friedman et al. [17] have flown a similar experiment in a satellite with a more favorable orbit, and their results have been published (Rawcliffe et al. [42]).

Inversion problems in measuring atmospheric parameters date back 35 years to the "Umkehr" method for determining the distribution of atmospheric ozone (Götz [20]). However, deduction of ozone by this method is not completely satisfactory. Recently Mateer [36] has analyzed the Umkehr method in greater detail than previous workers, and has contributed significantly to the understanding of inversion processes and their significance.

The methods proposed for determining the vertical temperature profile are intended for direct meteorological application. Vast areas of the earth are without radiosonde observations. The satellites can fill the gaps which exist. At the same time, this method is limited to the atmosphere above clouds. Nevertheless, most clouds are limited to the region below 700 mb.; with adequate surface information, complete soundings can be inferred by interpolation. Ozone information has no immediate meteorological application, and satellite observations should be regarded as experimental in nature.

## 2. GENERAL CONSIDERATIONS

The response of a satellite-borne spectrometer will be a function, usually linear and determinable by calibration, of the radiance of the source, integrated over frequency and angular view of the instrument, and weighted by the spectral and angular characteristics of the instrument. However, the radiance is related to the temperature profile and the optical properties of the atmosphere. At a single frequency $\nu$, the radiative transfer equation (Chandrasekhar [4], and Elsasser and Culbertson [12]) states that, for a plane-parallel atmosphere, which contains no scatterers, and which meets the requirement of local thermodynamic equilibrium,

$$d\{I(\nu,\theta)\}=\{-I(\nu,\theta)+B[\nu,T(z)]\}k(\nu)\rho(z)\sec\theta dz, \quad (1)$$

where $I(\nu,\theta)$ is the radiance at $\nu$ and in the direction $\theta$ from the local vertical, $k(\nu)$ is the absorption coefficient of the absorbing gas, $\rho(z)$ is the density of that gas, $B(\nu, T)$ is the Planck radiance at $\nu$ and the temperature $T$, and $z$ is the height in the local vertical; $T$ is, of course, expressed as a function of $z$.

Assume now that the instrument observes in a narrow cone in the local vertical so that everywhere in this cone $\sec\theta\approx 1$. Through the hydrostatic equation the variable $z$ can be transformed to pressure, so that $\rho dz=-q/gdp$, where $q$ is the mass mixing ratio of the absorbing gas and $g$ is gravitational acceleration, assumed constant at 980 cm./sec.$^2$ If the lower boundary is assumed to be black, equation (1) can then be written in the integral form

$$I(\nu,0)=\epsilon(\nu)B[\nu,T(p_0)]\exp\left[-\frac{q}{g}\int_0^{p_0}k(\nu,p)dp\right] +\frac{q}{g}\int_0^{p_0}B[\nu,T(p)]\exp\left[-\frac{q}{g}\int_0^{p}k(\nu,p)dp\right]k(\nu,p)dp, \quad (2)$$

where the subscript 0 refers to the lower boundary. This form of the equation shows the two components of the radiance: that arising from the surface and attenuated by the atmosphere; and that arising from the atmosphere itself.

It is convenient to simplify the notation by introducing the fractional transmittance

$$\tau(\nu,p)=\exp\left[-\frac{q}{g}\int_0^{p}k(\nu,p)dp\right] \quad (3)$$

of the beam between the level $p$ and the effective top of the atmosphere. Then (2) becomes,

$$I(\nu,0)=B[\nu,T(p_0)]\tau(\nu,p_0)-\int_1^{\tau(\nu,p_0)}B[\nu,T(p)]d\tau(\nu,p). \quad (4)$$

Equation (4) expresses radiance for a single wavelength; however, an instrument can distinguish only finite bandwidths. The measured instrument radiance in normalized form for a spectrometer is

$$I(\nu^*, 0)=\int_{\nu_1}^{\nu_2} w(\nu^*-\nu)I(\nu, 0)d\nu\Big/\int_{\nu_1}^{\nu_2} w(\nu^*-\nu)d\nu$$

$$=\left\{\int_{\nu_1}^{\nu_2} w(\nu^*-\nu)B[\nu, T(p_0)]\tau(\nu, p_0)d\nu\right.$$

$$-\int_{\nu_1}^{\nu_2}\int_0^{p_0} w(\nu^*-\nu)B[\nu, T(p)]$$

$$\left.\frac{\partial\tau(\nu,p)}{\partial p}dpd\nu\right\}\Big/\int_{\nu_1}^{\nu_2} w(\nu^*-\nu)d\nu, \quad (5)$$

where $w(\nu)$ is the spectrometer slit function and $\nu_1$, $\nu_2$ its limiting frequencies. A filter radiometer would, on the other hand, involve an inner product rather than a convolution product.

Equation (5) is hopelessly complicated. However, as pointed out by Elsasser [11], if the spectral interval $\nu_1$ to $\nu_2$ is small, then $B(\nu,T)$ varies little and is linear in the interval. It can, therefore, be replaced by its value $B(\bar{\nu},T)$ at a properly defined mean frequency $\bar{\nu}$, and factored out of the integral with respect to $\nu$. It becomes necessary to define the mean transmittance and its partial derivative by

$$\tau(\nu^*, p)=\frac{\int_{\nu_1}^{\nu_2} w(\nu^*-\nu)\tau(\nu, p)d\nu}{\int_{\nu_1}^{\nu_2} w(\nu^*-\nu)d\nu} \quad (6a)$$

and

$$\frac{\partial\tau(\nu^*, p)}{\partial p}=\frac{\int_{\nu_1}^{\nu_2} w(\nu^*-\nu)\,\frac{\partial\tau(\nu,p)}{\partial p}\,d\nu}{\int_{\nu_1}^{\nu_2} w(\nu^*-\nu)d\nu}. \quad (6b)$$

In the spectrometer discussed in this series of papers the spectral intervals are narrow (about 5 cm.$^{-1}$) and the slit functions $w(\nu)$ are symmetric and triangular. Therefore, for this particular instrument one may set $\nu^*$ equal to the mean frequency $\bar{\nu}$ and use (6a) and (6b) to rewrite (5) in the form

$$I(\bar{\nu}, 0)=B[\bar{\nu}, T(p_0)]\tau(\bar{\nu}, p_0)-\int_1^{\tau(\bar{\nu}, p_0)} B[\bar{\nu}, T(p)]d\tau(\bar{\nu},p). \quad (7)$$

Equations (4) and (7) are identical in form, but the latter contains the approximation $B(\bar{\nu},T)$ and introduces a mean transmittance. The step in going from one equation to the other is not trivial, but yields physically realizable functions.

Although it is not necessary in the discussion to follow, it will be assumed that the transmittance in all spectral intervals to be considered is zero at the surface, so that the first term on the right in (4) and (7) becomes zero. This is done to simplify the mathematics; however, in practice the equation can be used in the form of equation (7), as will become evident.

It is now apparent that the purpose of this investigation is to solve for the function $B(\bar{\nu}, T(p))$ in the second term on the right in (7), knowing the radiance and the transmittance. However, because there is a multiplicity of frequencies at which the observations are made, the Planck radiance is different in each equation, depending upon the frequency. It thus becomes vital to eliminate the frequency dependence in this function. In the microwave region the Rayleigh-Jeans law holds so that $B(\nu,T)=2\nu^2ckT$; in the region of the 4.3-micron carbon dioxide band Wien's law holds, so that $B(\nu,T)=2h\nu^3c^2\cdot$ exp $(-hc\nu/kT)$; in the vicinity of the 15-micron band neither approximation holds and one is required to linearize the Planck radiance in the form

$$B[\nu, T(p)]=\alpha(\nu)B[\nu_r, T(p)]+\beta(\nu), \quad (8)$$

where the subscript $r$ indicates a fixed reference frequency which is chosen near the middle of the range of frequencies. This approximation holds only over a limited part of the spectrum such as one might find in the 15-micron band. Of course there are alternatives to this form (see e.g. Marchuk [35], and Malkevitch and Tamarskii [34]), but in the present study (8) is the preferred approximation.

Equation (7), with the several limitations stated, may now be written

$$\frac{I(\nu, 0)-\beta(\nu)}{\alpha(\nu)}=-\int_0^{t_0} B[\nu_r, T(t)]\,\frac{d\tau(\nu, t)}{dt}\,dt, \quad (9)$$

where $\bar{\nu}$ is written as $\nu$ for convenience, and where $t$ is a general independent variable to which pressure can be transformed; however, it has been found generally that log $p$ is probably a suitable transformation for this problem. Equation (9) is a Fredholm equation of the first kind,

$$g(\nu)=\int_0^{t_0} K(\nu, t)f(t)dt, \quad (10)$$

where the kernel $K(\nu,t)$ is the derivative of the known transmittance and the indicial function $f(t)=B[\nu_r,T(t)]$ is to be recovered through the application of the observed quantity

$$g(\nu)=[I(\nu, 0)-\beta(\nu)]/\alpha(\nu).$$

## 3. THE NATURE OF THE KERNEL

In the infrared and microwave parts of the spectrum all absorption by the gases of the atmosphere is caused by spectral lines resulting from transitions between bound states of the molecules. At any frequency there is absorption by a line or lines and by a quasi continuum caused by the wings of nearby and distant lines. In the 15-micron band there are a number of individual bands of carbon dioxide which contribute significantly to the absorption. The most important of these is the $\nu_2$ funda-

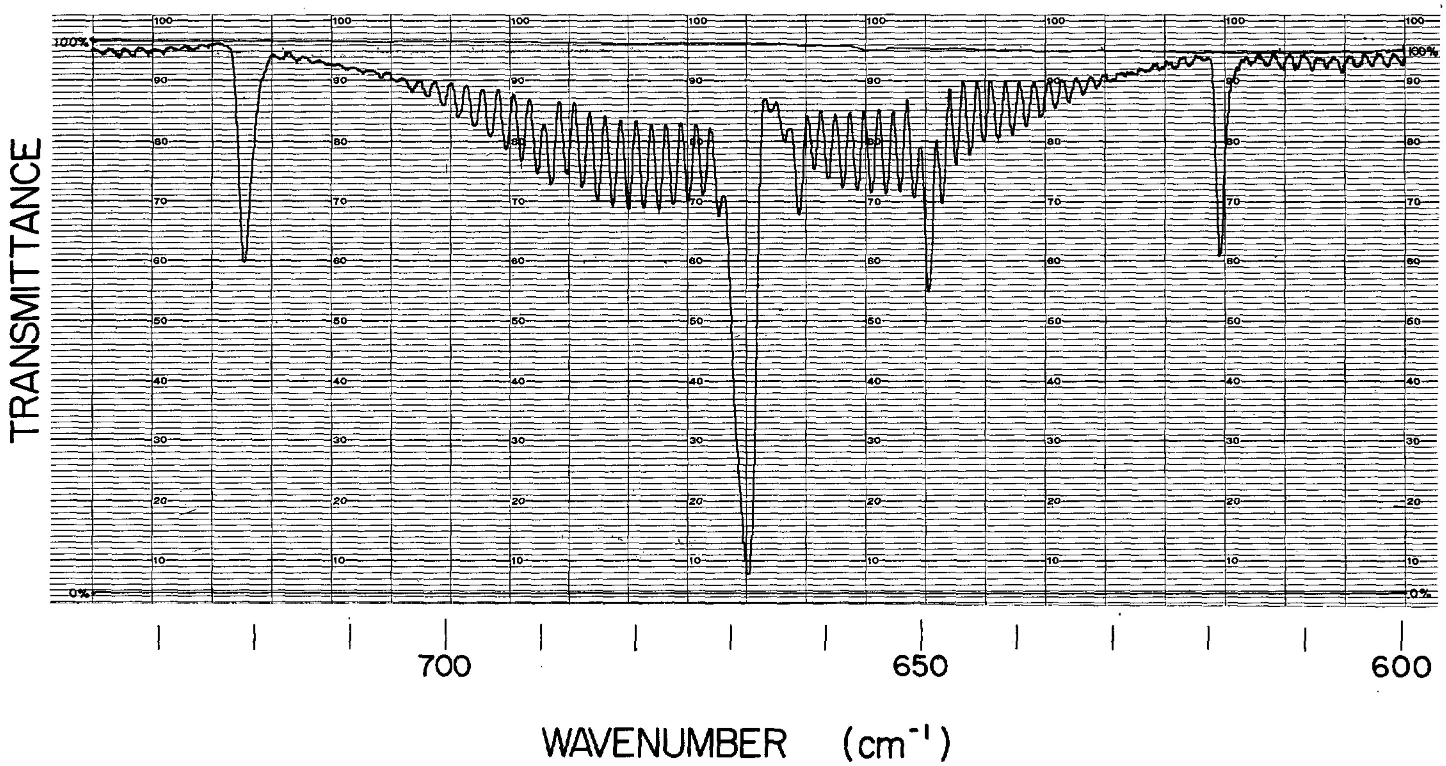



FIGURE 1.—A medium-high resolution spectrum of the 15-micron carbon dioxide band. This spectrum was obtained from a 10-cm. path of pure carbon dioxide at 63 mb. and 38° C. The strong $Q$ branch at 667 cm.$^{-1}$ flanked by the $P$- and $R$-branch lines dominate the absorption. The weaker $Q$ branches at 618, 648, 662, 688, and 721 cm.$^{-1}$ appear in this figure.

mental vibration-rotation band. In addition there are a number of weaker bands caused by vibrational transitions between excited states (the so called "hot" bands) and by molecules containing the less abundant isotopes. In each of these bands there is a strong $Q$ branch located at the center of the band with $P$-branch and $R$-branch lines almost equally spaced on each side of the band center. Figure 1 shows a medium-high resolution spectrum of this band obtained with a spectrometer. The strong $Q$ branch of the $\nu_2$ fundamental at 667.4 cm.$^{-1}$ shows the maximum absorption, resulting from many nearly superposed lines. The $Q$ branches of five other bands can be seen in this figure at 618, 648, 662, 688, and 721 cm.$^{-1}$, although the $P$ and $R$ branches of all but the first and last of these are too weak to show. The $P$-branch and $R$-branch lines in the $\nu_2$ fundamental band are seen to be spaced regularly in a manner suggesting an Elsasser [10] band. In other molecules, such as water vapor, the lines are spaced irregularly and have irregular intensities in contrast with the spectrum seen in figure 1 for carbon dioxide.

In the atmosphere the transmittance, which is a determining factor in the radiance to be observed from a satellite at any frequency, depends upon the spectral interval observed. For example, the intervals employed in the infrared spectrometer to be discussed later have bandwidths of about 5 cm.$^{-1}$ In the microwave region, where higher resolution is theoretically possible, portions of lines can be observed.

Through most of the atmosphere (up to about 50 km.) the broadening of spectral lines is dominated by collisions; above that level Doppler broadening of the lines dominates. Thus, one finds in the meteorologically significant parts of the atmosphere that lines have Lorentz shapes

$$k(\nu)=\frac{S}{\pi}\frac{\alpha}{(\nu-\nu_0)^2+\alpha^2}, \tag{11}$$

where $S$ is the line intensity $(S=\int_0^\infty k(\nu)d\nu)$, $\alpha$ is the line halfwidth, and $\nu_0$ is the frequency of the line center.

Now let us postulate the transmittance, and thereby components of the kernel function, for different conditions, as follows:

1. An Elsasser band, where the bandwidth is equal to at least one cycle.
2. A narrow spectral interval in the far wing of the line $(k(\nu)=S\alpha/\pi(\nu-\nu_0)^2)$.
3. Near the center of the line (Equation (11) holds strictly).
4. A spectral interval in which the mass absorption coefficient is constant with respect to height in the atmosphere. (This condition is not found in the infrared or microwave region of the spectrum, except in isothermal regions where Doppler broadening dominates.)

We may now calculate the transmission functions for an isothermal atmosphere in which the usual dependence of line widths

$$\alpha=\alpha_0\frac{p}{p_0}\sqrt{\frac{T_0}{T}}$$

holds; here, $\alpha_0$ is the half width at half intensity at NTP and $T_0$ and $p_0$ are NTP. The resulting set of functions $d\tau(\nu, \log p)/d(\log p)$ is shown in figure 2. It is seen that the function for the far wing of the line is more peaked than for any other condition given above; because of the pressure dependence of the line width, the function for the near wing of the line converges to that of the far wing at lower pressures. The Elsasser band function is noticeably broader at its half maximum point, but the difference between an Elsasser band and the extreme far wing of the line is not so great as one might imagine. For example, the width at half maximum for the wing is approximately 8 km., whereas for the Elsasser band it is about 12 km. Thus, there is a small but not striking advantage to high resolution in the spectrum from the standpoint of narrowing the function $d\tau(\nu, \log p)/d(\log p)$ in the atmosphere. The great advantage in high resolution is that it allows one to observe at higher levels of the atmosphere. The function for a 5 cm.$^{-1}$ interval centered in the $Q$ branch of the 15-micron band will differ somewhat from the examples shown in figure 2. The reason for this is that the bulk of the absorption is concentrated in a limited part of the 5 cm.$^{-1}$ interval and other parts of this interval are at the minima between the branches, as seen in figure 1.

In practice it is possible to observe the spectrum only at discrete intervals and the kernel is therefore not a continuous function of $\nu$. Consequently, we are no longer dealing with a single equation, but rather with a system of equations, and the number of independent pieces of information to be gained in the indicial function is equal to or less than the number of equations. For example, in the balloon model of the instrument which we are considering, there are six spectral intervals, centered at 669.0, 677.5, 691.0, 697.0, 703.0, and 709.0 cm.$^{-1}$ The first of these intervals was chosen because it is the most absorbent region of the 15-micron band, which allows one to see as high as possible into the stratosphere. The second interval is at the maximum of the $R$ branch, which absorbs considerably less than the $Q$-branch interval. The other four intervals are spaced so that they will meet

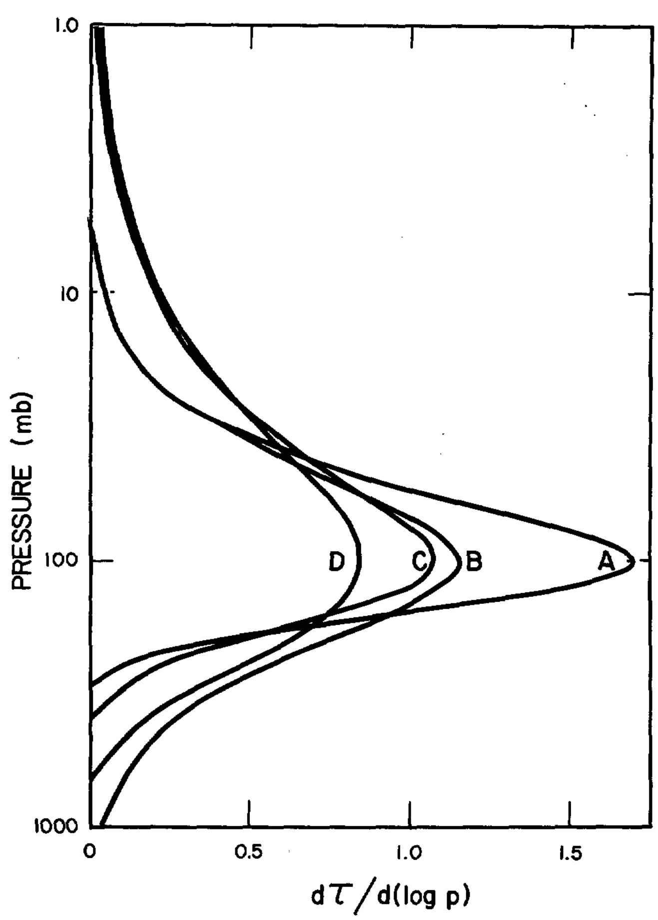



FIGURE 2.—Hypothetical weighting functions $d\tau/d(\log p)$, with maximum values at 100 mb., versus log $p$ for the following conditions: (A) the far wing of a line; (B) near the line center ($\nu-\nu_0=\alpha$ at 100 mb.); (C) an Elsasser band; (D) constant mass absorption coefficient.

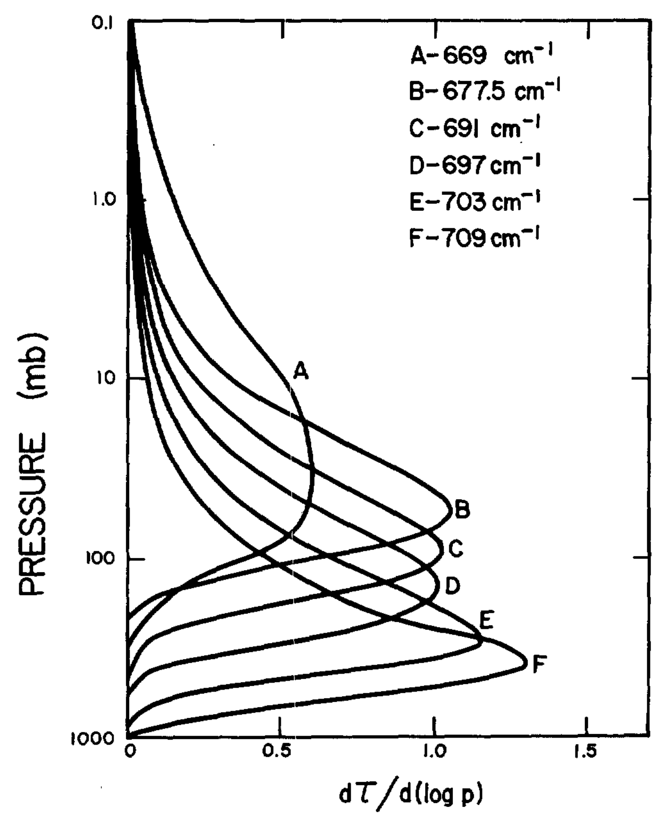



FIGURE 3.—The six components of the kernel $d\tau(\nu, p)/d(\log p)$, versus log $p$, in the 15-micron carbon dioxide band.

the conditions given in the next section; that is, the functions $d\tau(\nu, \log p)/d(\log p)$ overlap, but maintain a considerable degree of independence. Furthermore, the function in the last of these intervals goes to zero at the surface in a standard atmosphere. Figure 3 shows the functions for these six intervals for the U.S. Standard Atmosphere [53].

## 4. DETERMINATION OF THE TEMPERATURE PROFILE

The curves shown in figure 3 may be considered as weighting functions for the Planck radiance in equation (9). These curves show from what part of the atmosphere the outgoing radiance arises, but the quantitative value depends upon the product of these curves and the shape of the Planck function with respect to the independent variable. It is vital that the weighting functions overlap somewhat in order that one can obtain enough data to define the temperature profile adequately. One may consider two extremes; weighting functions which have no significant overlap and weighting functions whose overlap is nearly complete. In the first case the solution is trivial, but also meaningless because it represents a mean temperature over the gross features of the atmosphere defined only by the integral form of the radiative transfer equation. In the second case the errors of measurement exceed the ability of the weighting functions to discriminate between the levels of the atmosphere from which the radiation is arising. Aside from the errors of measurement, it is shown by Twomey in the following paper of this series that the number of *independent* pieces of information regarding the temperature sounding is sharply limited.

It is known (cf., Baker et al. [2], Courant and Hilbert [5] (pp. 159–160), Mayers [37], Kunz [31] (pp. 353–355)) that no unique solution $f(t)$ exists to equation (10)—in fact, no solution may exist at all. Furthermore, $g(\nu)$ is measured at only $n$ discrete values of $\nu$, and so the indicial function $f(t)$ must be approximated by some explicit closed form with at most $n$ undetermined coefficients or $n$ undetermined parameters. Thus there are an infinite number of possible approximate solutions. For example, Wark [54], Yamamoto [55], Twomey and Howell [52], King [29], Malkevitch [33], Malkevitch and Tamarskii [34], Fleming and Wark [14], [15], and Alishouse et al. [1] have chosen line segments, polynomials, slabs, and empirical functions. Each of these gives a reasonable approximation to the sounding. On the other hand, most solutions are deficient in one way or another, particularly when the number of equations is small. The atmosphere is known to contain discontinuities of slope, particularly at the tropopause. The polynomial solutions are unable to reproduce these sharp corners; line segments and slabs require that part of the information be used to determine the pressure positions of the corners and leave few data for determining the temperature. The successive use respectively, of the first two solutions can overcome the latter difficulty. However, the empirical orthogonal functions (Lorenz [32], Obukhov [40], Holmström [23], Alishouse et al. [1]) based upon measured temperature profiles have, by the physical nature of their derivation, the inherent qualities of the temperature profiles and are thus able to reproduce the profiles with greater fidelity and more efficient use of the data.

Once the form of the indicial function $f(t)$ has been decided upon, one can reduce the integral equation (10) to a system of linear algebraic equations by applying an appropriate numerical quadrature formula. For example, assume that the indicial function is expressed by

$$f(t)=\sum_{j=1}^{n} c_j\phi_j(t), \tag{12}$$

where the $\phi_j(t)$ may be classical orthogonal polynomials, powers of $t$, trigonometric functions, or empirical orthogonal functions. Now (10) becomes

$$g(\nu_i)=\sum_{j=1}^{n} c_j \int_0^{t_0} K(\nu_i, t)\phi_j(t)dt, \qquad i=1, \ldots, n, \tag{13}$$

which, after applying the numerical quadrature, may be written in the matrix form

$$\mathbf{g}=\mathbf{A}\mathbf{c}, \tag{14}$$

where $\mathbf{g}$ is the vector expression of the observed quantities $g(\nu_i)$, $\mathbf{A}$ is the matrix whose elements are given by the integrals in (13), and $\mathbf{c}$ is the vector of undetermined coefficients. The solution vector $\mathbf{c}$ is given directly by

$$\mathbf{c}=\mathbf{A}^{-1}\mathbf{g}, \tag{15}$$

where $\mathbf{A}^{-1}$ is the inverse of the matrix $\mathbf{A}$.

Disaster strikes quickly when (15) is used as a solution. This becomes evident when the number $n$ of equations is large; when $n=3$, for example, reasonable solutions seem to result, but when $n=6$ the solution deviates from the true sounding by an amount which is completely unacceptable for meteorological purposes. This can best be illustrated by a solution of connected line segments; the formulaton of this solution is not given here because it will not be employed further. Figure 4 shows the U.S. Standard Atmosphere [53] from which the radiance values were calculated for the six intervals listed in section 3 by employing equation (7) and the weighting functions shown in figure 3. These "exact" values of radiance were applied to (15) and the solution marked $\gamma=0$ resulted; the oscillations of this solution carry the end points of the upper two line segments far beyond the limits of this figure. This solution is absurd.

The instability of this solution can be traced to the following sources of error:

a) The approximation to the Planck function given by (8),
b) The errors arising from the numerical quadrature

used for calculating the radiances from (7) and for calculating the elements of the matrix $\mathbf{A}$ in (15),

c) Round-off errors.

Thus there are errors in the matrix $\mathbf{A}$ as well as in the input vector $\mathbf{g}$, and together they are responsible for the erratic behavior of the direct solution (see Fleming and Wark [15]).

In the papers by Phillips [41], Twomey [50], [51], Twomey and Howell [52], and Fleming and Wark [14], [15] the means of ameliorating the instability manifest in the erratic solutions has been thoroughly discussed. In the second paper of this series Twomey further analyzes the causes of the instability of this problem.

From these studies comes the solution

$$\mathbf{c}=(\mathbf{A}^T\mathbf{A}+\gamma\mathbf{H})^{-1}(\mathbf{A}^T\mathbf{g}+\gamma\mathbf{h}), \tag{16}$$

where $\mathbf{A}^T$ is the transpose of $\mathbf{A}$, $\gamma$ is the smoothing parameter, $\mathbf{H}$ is the smoothing matrix and $\mathbf{h}$ is a bias vector which is a gross a priori estimate of the solution vector $\mathbf{c}$. When the solution employs the bias vector the matrix $\mathbf{H}$ becomes the identity matrix $\mathbf{I}$; otherwise, $\mathbf{h}\equiv\mathbf{0}$, and (16) has the form

$$\mathbf{c}=(\mathbf{A}^T\mathbf{A}+\gamma\mathbf{H})^{-1}\mathbf{A}^T\mathbf{g}. \tag{17}$$

Equation (16) minimizes the deviation of the solution vector $\mathbf{c}$ from the bias vector $\mathbf{h}$. However, the deviation of the solution vector $\mathbf{c}$ may be also minimized with respect to its own mean. On the other hand, this equation might represent a minimization of the change in slope of the solution. The $\mathbf{H}$ matrix in (17) for these cases is given implicitly in Phillips [41], and explicitly in Twomey [50], [51] and Fleming and Wark [14]. An estimate for $\gamma$ is found by pragmatic devices such as those used in the following section or in the papers just cited.

When (17) is applied to the standard atmosphere, the solution marked $\gamma=10^{-5}$ in figure 4 results. This solution is deceptively good because of the selection of the end points of the line segments at the known lapse rate discontinuities; this cannot be done in practice.

As mentioned previously, the empirical orthogonal functions are found to be superior to other forms of solution. From the discussion given in Alishouse et al. [1], the deviations from a mean sounding are expanded in the empirical functions. Because the solution is in terms of deviations, the bias vector $\mathbf{h}$ is the zero vector in (16), and the solution becomes (17) with the matrix $\mathbf{H}$ the identity matrix $\mathbf{I}$. This form of the solution is used in the next section of this paper.

## 5. RESULTS OF COMPUTATION

From the radiosonde observations employed by Alishouse et al. [1] to develop a set of empirical orthogonal functions, four of these soundings, which are extrapolated to 0.1 mb., have been selected for analysis. For each sounding, the radiances in the six spectral intervals were calculated from (7), and the results applied to (17). The

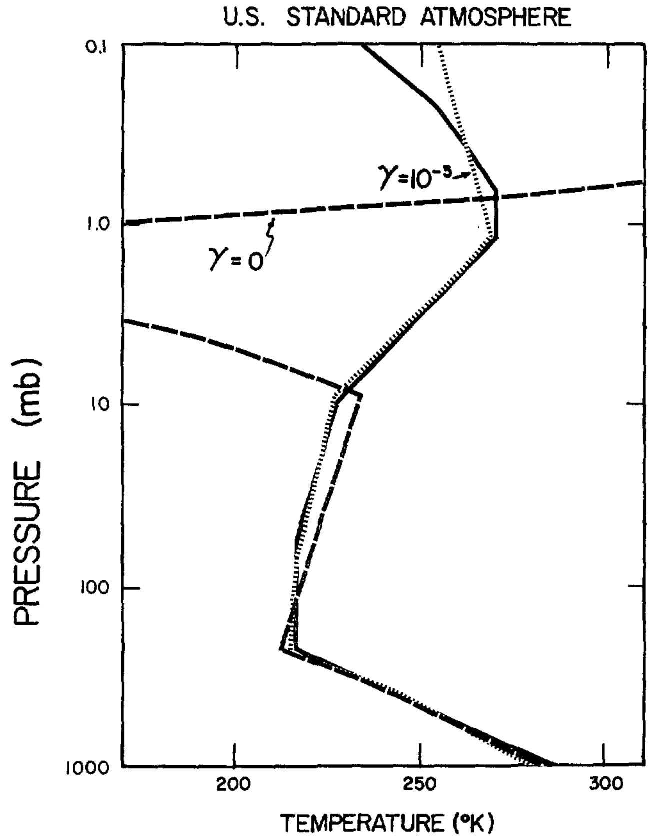
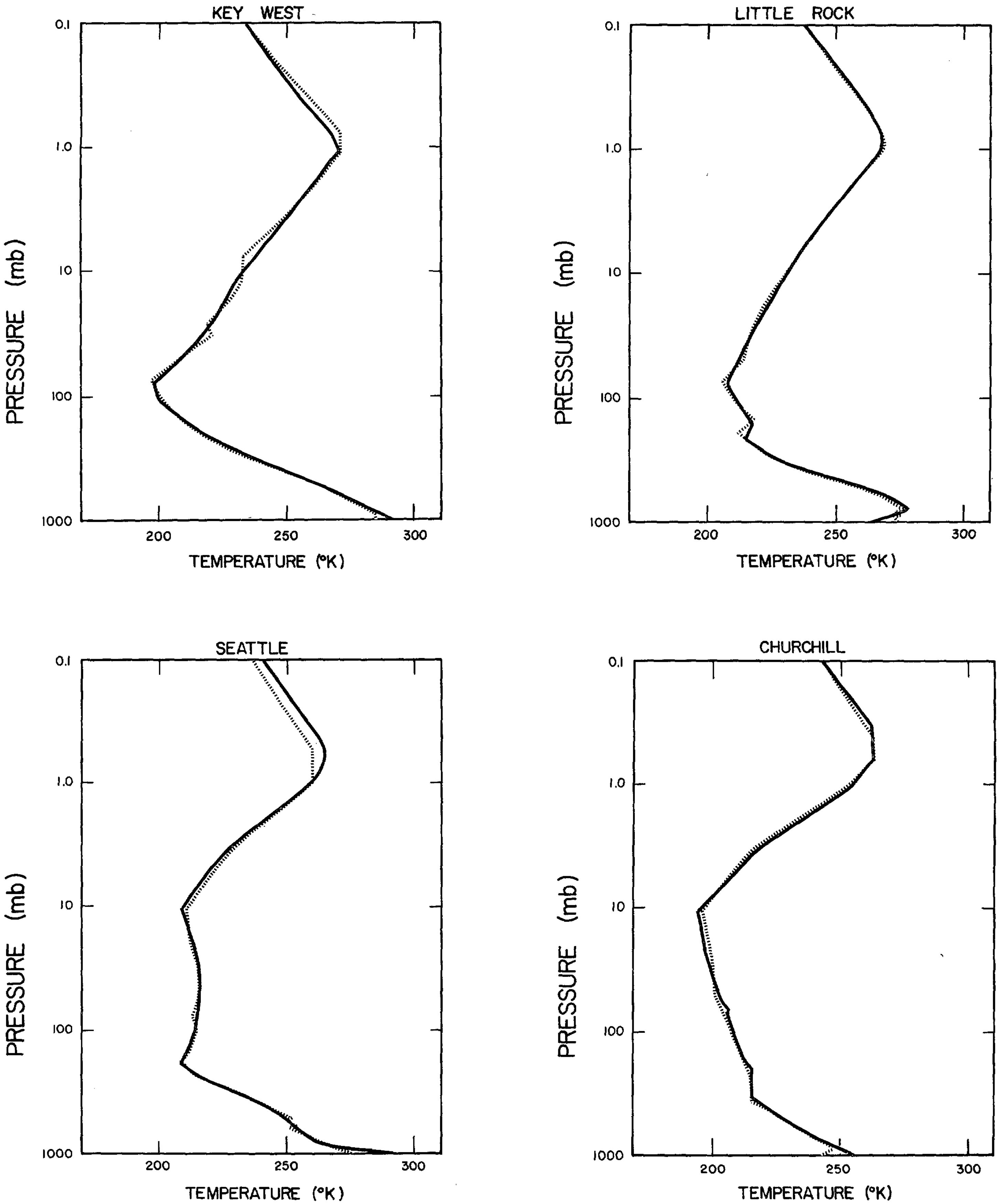



FIGURE 4.—Solutions to the inverse problem for the U.S. Standard Atmosphere [53], shown by the dotted line, using "exact" radiance values. The direct solution, marked $\gamma=0$, and the smoothed solution, marked $\gamma=10^{-5}$, were determined by sequences of line segments whose end points were selected at the known turning points.

original soundings and the solutions are shown in figures 5 to 8. Figure 3 clearly shows that these solutions are meaningful only between about 700 mb. and 5 mb. The good agreement in figures 5 to 8 above 5 mb. is fortuitous because of the uniform extrapolation applied to the radiosondes used in generating the empirical functions.

It is readily apparent that the same set of empirical functions does not reproduce each of the soundings with equal fidelity. The cause of this does not lie in the use of empirical functions, but rather in the particular set used; these functions were derived from 106 soundings over the area from Curaçao to Alert, NWT, and from Bermuda to Shemya, Alaska on January 14, 1961. These included almost the complete variety of soundings which are found, from the Tropics to extremes of the winter Arctic. It is obvious that a single set of six empirical functions cannot reproduce all soundings. It is equally obvious that this deficiency can be overcome by employing several sets of functions which would represent different seasons and geographical areas.

Until now no quantitative consideration has been given to the effects of the errors of the radiance measurements upon the temperature profiles obtained from (17). The




FIGURES 5–8.—Solutions to the inverse problem for Key West, Little Rock, Seattle, and Churchill, respectively. The solutions used empirical orthogonal functions and the smoothing parameter $\gamma=10^{-4}$, and were derived from "exact" radiance values. The dotted and solid lines are the actual and deduced soundings, respectively.

magnitude of the radiances in the six channels is approximately 50 ergs/(cm.$^2$ sec. strdn. cm.$^{-1}$). We now select four groups of random errors, each group having 110 sets of six errors, with each group of 660 having root mean square values $\sigma=$ 0.25, 0.50, 1.00, and 2.00 ergs/(cm.$^2$ sec. strdn. cm.$^{-1}$); these groups represent measurement errors of about ½, 1, 2, and 4 percent, respectively. By adding these to the "exact" radiance values calculated from (7) and carrying out the solutions from (17) for the resulting sets of radiances, an estimate can be made of the errors to be expected in the temperature profiles.

Because the solutions are in terms of the Planck radiance, $B[\nu_r, T(t)]$, the expected mean errors in temperature must be evaluated from these radiances. It is readily apparent that the radiances must be weighted by the relative contributions from the different levels of the atmosphere as determined by the components of the kernel. Thus, one may write

$$\overline{B}\pm\overline{\Delta B}\equiv\overline{g}\pm\overline{\Delta g}=\frac{1}{110}\sum_{k=1}^{110}\frac{1}{\int_0^{t_0}\left[\sum_{i=1}^{6}\frac{d\tau(\nu_i,t)}{dt}\right]dt}$$
$$\left\{\int_0^{t_0}B_C^{[k]}(t)\left[\sum_{i=1}^{6}\frac{d\tau(\nu_i,t)}{dt}\right]dt\pm\int_0^{t_0}|B_C^{[k]}(t)-B_A(t)|\left[\sum_{i=1}^{6}\frac{d\tau(\nu_i,t)}{dt}\right]dt\right\}, \quad (18)$$

where $B_C^{[k]}(t)$, $k=1, \ldots, 110$, and $B_A(t)$ are the calculated and actual Planck radiances at the reference wave number $\nu_r$.

The 110 sets of random errors introduced into (17) and applied to (18) constitute a sufficiently large sample to consider $\overline{B}$ and $\overline{\Delta B}$ as adequate for a transformation to the expected mean weighted temperature and its corresponding variance for a single sounding and a single variance in the observational errors. The mean temperature inferred from (18) is given by the Planck relation,

$$\overline{T}=\frac{hc\nu_r}{k\log\left(\frac{2h\nu_r^3c^2}{\overline{B}}+1\right)}, \quad (19)$$

and its variance by,

$$\overline{\Delta T}=\frac{\overline{\Delta B}}{\partial\overline{B}/\partial T}=\frac{\overline{\Delta B}}{\overline{B}}\left[\frac{2\nu_r^2ck\overline{T}^2}{2h\nu_r^3c^2+\overline{B}}\right]. \quad (20)$$

The soundings shown in figures 5–8 were subjected to the above analysis. From a small sample of "errors" a suitable value of $\gamma$ for each value of $\sigma$ was determined on the basis of minimizing $\overline{\Delta B}$; these values of $\gamma$ were then applied to the random sample of 110 sets of errors for each $\sigma$. The results are shown in table 1.

It is obvious that one cannot compensate increasingly large errors of measurement by increased smoothing. As $\gamma$ increases, the elements of the matrix $\gamma\mathbf{H}$ in (17) approach the magnitude of the elements of $\mathbf{A}^T\mathbf{A}$. When this condition exists, the nature of the solution of (17) is dictated by the matrix $\mathbf{H}$; in the extreme, the solution employing empirical orthogonal functions will be the mean sounding displaced by a constant value. The value of $\gamma$ used in table 1 for $\sigma=2.0$ ergs/(cm.$^2$ sec. strdn. cm.$^{-1}$) makes the diagonal elements of $\gamma\mathbf{H}$ roughly one tenth the value of the diagonal elements of $\mathbf{A}^T\mathbf{A}$. Therefore, any sounding which does not resemble the mean sounding will be significantly distorted. It can be seen that Little Rock is more nearly like the mean sounding than are the other three, because $\overline{\Delta B}$ is smaller for $\sigma=2.0$ ergs/(cm.$^2$ sec. strdn. cm.$^{-1}$), even though it is the second largest for $\sigma=0$, where $\gamma$ is very small.

From table 1 it should be apparent that the errors of measurement must be minimized to the greatest degree possible. Errors exceeding about $\sigma=0.5$ erg/(cm.$^2$ sec. strdn. cm.$^{-1}$) lead to results which do not meet the requirements of meteorology.

The value of $\gamma$ which is appropriate to a solution of (17) depends mainly upon the random errors of measurement, as can be seen in table 1. This places a specific requirement upon the instrument. A calibration source is needed on the satellite, not only to establish the relation between the source radiances and radiometric outputs, but also, from many consecutive readings, to determine the root mean square errors of radiance measurement.

## 6. CONCLUSION

No solution is meaningful at heights where the ensemble of weighting functions has insignificant information

TABLE 1.—*Comparative results of applying random errors of observation of varying magnitude to the deduction of temperature profiles. The columns marked "maximum" are for the fifth largest value. The units for $\sigma$, $\overline{B}$, $\overline{\Delta B}$, and Max. $\Delta B$ are ergs /(cm.$^2$ sec. strdn. cm.$^{-1}$); the units for $\overline{T}$, $\overline{\Delta T}$, and Max. $\Delta T$ are °K.*

| $\sigma$ | $\gamma$ | KEY WEST | | | | LITTLE ROCK | | | | SEATTLE | | | | CHURCHILL | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | $\overline{B}\pm\overline{\Delta B}$ | $\overline{T}\pm\overline{\Delta T}$ | Max. $\Delta B$ | Max. $\Delta T$ | $\overline{B}\pm\overline{\Delta B}$ | $\overline{T}\pm\overline{\Delta T}$ | Max. $\Delta B$ | Max. $\Delta T$ | $\overline{B}\pm\overline{\Delta B}$ | $\overline{T}\pm\overline{\Delta T}$ | Max. $\Delta B$ | Max. $\Delta T$ | $\overline{B}\pm\overline{\Delta B}$ | $\overline{T}\pm\overline{\Delta T}$ | Max. $\Delta B$ | Max. $\Delta T$ |
| 0 | $10^{-4}$ | 47.59±0.96 | 224.65±1.01 | 0.96 | 1.01 | 47.39±0.93 | 224.43±0.98 | 0.93 | 0.98 | 43.84±0.69 | 220.60±0.76 | 0.69 | 0.76 | 35.13±0.86 | 210.36±1.08 | 0.86 | 1.08 |
| 0.25 | 0.025 | 47.59±1.80 | 224.65±1.90 | 2.50 | 2.63 | 47.39±1.21 | 224.43±1.28 | 1.69 | 1.79 | 43.84±1.60 | 220.60±1.77 | 2.47 | 2.73 | 35.13±1.71 | 210.36±2.14 | 2.24 | 2.81 |
| 0.5 | 0.050 | 47.60±2.01 | 224.66±2.12 | 2.85 | 3.00 | 47.40±1.54 | 224.44±1.63 | 2.55 | 2.69 | 43.85±1.89 | 220.61±2.09 | 3.27 | 3.61 | 35.14±1.96 | 210.38±2.46 | 2.89 | 3.63 |
| 1.0 | 0.150 | 47.61±3.04 | 224.67±3.20 | 4.63 | 4.88 | 47.41±2.13 | 224.46±2.25 | 3.62 | 3.82 | 43.86±2.45 | 220.62±2.70 | 4.47 | 4.93 | 35.15±2.79 | 210.39±3.50 | 4.65 | 5.84 |
| 2.0 | 0.400 | 47.63±4.42 | 224.69±4.66 | 6.36 | 6.70 | 47.43±2.81 | 224.48±2.97 | 4.38 | 4.63 | 43.88±3.05 | 220.64±3.37 | 5.25 | 5.79 | 35.17±4.14 | 210.41±5.20 | 6.25 | 7.84 |

content. Thus, figure 3 indicates that the functions shown there are significant only between about 700 mb. and 5 mb. With the spectrometer mentioned earlier in this paper, and described in the third paper of this series, the upper level of significance cannot be extended; however, by a slight rearrangement of four channels and the addition of a seventh channel which is partly transparent down to the surface, the entire sounding can be obtained. With this new arrangement, both terms on the right in (7) must be used, and the seven channels must be supplemented with an eighth one at 899 cm.$^{-1}$ to determine the surface temperature.

Although the main problem has been discussed here in some detail, there are a number of other problems which have not been mentioned, and which are of varying degrees of difficulty.

(a) When there is a thick overcast, the solution is comparatively simple, requiring only a "stepping-down" process. The solution is, however, limited to the region above the cloud tops.

(b) When thin clouds or partly cloudy conditions exist, the solution is more difficult and is the subject of current investigation.

(c) The transmittances in the various channels are slightly dependent upon temperature, and therefore upon the solution itself. However, this can be solved by an iterative process.

(d) Water vapor contributes significantly to the transmittances in the lower levels of the atmosphere. This requires that a reasonable estimate of the total water vapor and its vertical distribution be made. However, the solution is not highly sensitive to the values of transmittance, so that only a gross error in the estimate of the water vapor would lead to significant errors in the deduction of the vertical temperature profile in the lower troposphere.

The authors feel that the feasibility of the determination of temperature soundings on a worldwide scale from satellite radiometric measurements in the infrared is fully demonstrated, and that a nearly complete technique exists to accomplish this.

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